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Poisson's Ratio for Hexagonal Crystals

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ARL-TR-424 March 1995

NOTICES

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REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. AGENCY USE ONLY *(Leave blank)*

2. REPORT DATE
March 1995

3. REPORT TYPE AND DATES COVERED
Technical Report

4. TITLE AND SUBTITLE
POISSON'S RATIO FOR HEXAGONAL CRYSTALS

5. FUNDING NUMBERS

6. AUTHOR(S)
Arthur Ballato

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
US Army Research Laboratory (ARL)
Electronics and Power Sources Directorate (EPSD)
ATTN: AMSRL-EP
Fort Monmouth, NJ 07703-5601

8. PERFORMING ORGANIZATION REPORT NUMBER
ARL-TR-424

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)

10. SPONSORING/MONITORING AGENCY REPORT NUMBER

11. SUPPLEMENTARY NOTES

12a. DISTRIBUTION/AVAILABILITY STATEMENT
Approved for public release; distribution is unlimited.

12b. DISTRIBUTION CODE

13. ABSTRACT *(Maximum 200 words)*

General expressions for Poisson's ratio are derived for hexagonal crystals; simplified forms are given for cases involving symmetry directions.

14. SUBJECT TERMS
Piezoelectric wurtzite structure; hexagonal

15. NUMBER OF PAGES
13

16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT
Unclassified

18. SECURITY CLASSIFICATION OF THIS PAGE
Unclassified

19. SECURITY CLASSIFICATION OF ABSTRACT
Unclassified

20. LIMITATION OF ABSTRACT
UL

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POISSON'S RATIO FOR HEXAGONAL CRYSTALS

Abstract

General expressions for Poisson's ratio are derived for hexagonal crystals; simplified forms are given for cases involving symmetry directions.

Introduction

Poisson's ratio, ν, is defined for isotropic media as the quotient of lateral contraction to longitudinal extension arising from application of a simple tensile stress; in most materials, this dimensionless number is positive. In crystals, ν takes on different values, depending on the directions of stress and strain chosen. The ratio finds application in a variety of areas of applied elasticity and solid mechanics, for example, as indication of the mechanical coupling between various vibrational modes of motion.

The maximum value of $\nu = +1/2$ is obtained in the incompressible medium limit, where volume is preserved; for ordinary materials, values of $+1/4$ to $+1/3$ are typical, but in crystals ν may vanish, or take on negative values. Analytical formulas for Poisson's ratio are expressed in terms of elastic constants. For the case of crystals of general anisotropy, these expressions are quite unwieldy, but for hexagonal crystals the symmetry elements reduce the complexity considerably.

Crystals of hexagonal symmetry include a number of the binary semiconductor systems with the piezoelectric wurtzite structure, such as GaN and AlN. These are becoming increasingly important for high technology applications. One of the most important representatives of this class is the family of poled electroceramics, including $BaTiO_3$, PZT, and related alloys. All hexagonal classes have the same elastic matrix scheme, so for our purposes it is not necessary to distinguish between the different point groups; the presence of piezoelectricity is neglected.

Expressions Relating Hexagonal Stiffnesses and Compliances

Relations for Poisson's ratio are most simply expressed in terms of the elastic compliances $[s_{\lambda\mu}]$. It is often the case, however, that the most accurate determinations of the elastic constants (resonator and transit-time methods) yield values for the stiffnesses $[c_{\lambda\mu}]$ directly; the conversion relations are given below. For the hexagonal system, the elastic stiffness and compliance matrices have identical form. Referred to the x_k axes as defined in the IEEE Standard, the matrices are:

$$\begin{matrix} c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\ c_{12} & c_{11} & c_{13} & 0 & 0 & 0 \\ c_{13} & c_{13} & c_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{66} \end{matrix} \qquad \begin{matrix} s_{11} & s_{12} & s_{13} & 0 & 0 & 0 \\ s_{12} & s_{11} & s_{13} & 0 & 0 & 0 \\ s_{13} & s_{13} & s_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & s_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & s_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & s_{66} \end{matrix}$$

Stiffness and compliance are matrix reciprocals; the four independent components of each are related by:

$$(c_{11} + c_{12}) = s_{33} / S\,; \qquad (c_{11} - c_{12}) = 1 / (s_{11} - s_{12})$$

$$c_{13} = - s_{13} / S\,; \qquad c_{33} = (s_{11} + s_{12}) / S$$

$$c_{44} = 1 / s_{44}\,; \qquad S = s_{33}(s_{11} + s_{12}) - 2\, s_{13}{}^{2}$$

In addition, one has the relation $s_{66} = 2(s_{11} - s_{12})$. The compliances are given in terms of the stiffnesses by:

$$(s_{11} + s_{12}) = c_{33} / C\,; \qquad (s_{11} - s_{12}) = 1 / (c_{11} - c_{12})$$

$$s_{13} = - c_{13} / C\,; \qquad s_{33} = (c_{11} + c_{12}) / C$$

$$s_{44} = 1 / c_{44}\,; \qquad C = c_{33}(c_{11} + c_{12}) - 2\, c_{13}{}^{2}$$

and $c_{66} = (c_{11} - c_{12})/2$. The equality of the 11 and 22 components together with the given relations between the 66, 11 and 12 components imply transverse isotropy; that is, all directions perpendicular to the unique 6-fold axis (i.e., in the basal plane), are elastically equivalent.

Definition of Poisson's Ratio for Crystals

Poisson's ratio for crystals is defined in general as $\nu_{ji} = s_{ij}' / s_{jj}'$, where x_j is the direction of the longitudinal extension, x_i is the direction of the accompanying lateral contraction, and the s_{ij}' and s_{jj}' are the appropriate elastic compliances referred to this right-handed axial set. It suffices to take x_1 as the direction of the longitudinal extension; then two Poisson's ratios are defined by the orientations of the lateral axes x_2 and x_3: $\nu_{21} = s_{12}' / s_{11}'$ and $\nu_{31} = s_{13}' / s_{11}'$. Application of the definition requires specification of the orientation of the x_k coordinate set with respect to the crystallographic directions, and transformation of the compliances accordingly.

Relations for Rotated Hexagonal Compliances - General

The unprimed compliances are referred to a set of right-handed orthogonal axes related to the crystallographic axes in the manner defined by the IEEE standard. Direction cosines a_{mn} relate the transformation from these axes to the set specifying the directions of the applied longitudinal extension (x_1), and the resulting lateral contractions (x_2 and x_3). General expressions for the transformed hexagonal compliances that enter the formulas for ν_{21} and ν_{31} are:

$$s_{11}' = s_{11}\,[a_{11}^2 + a_{12}^2]^2 + s_{33}\,[a_{13}^4] + (s_{44} + 2\,s_{13})\,[a_{13}^2][a_{11}^2 + a_{12}^2]$$

$$\begin{aligned} s_{12}' = {} & s_{11}\,[a_{11}\,a_{21} + a_{12}\,a_{22}]^2 + s_{33}\,[a_{13}^2\,a_{23}^2] + \\ & s_{44}\,[a_{13}\,a_{23}][a_{11}\,a_{21} + a_{12}\,a_{22}] + s_{12}\,[a_{11}\,a_{22} - a_{12}\,a_{21}]^2 + \\ & s_{13}\,[a_{23}^2\,[a_{11}^2 + a_{12}^2] + a_{13}^2\,[a_{21}^2 + a_{22}^2]] \end{aligned}$$

$$\begin{aligned} s_{13}' = {} & s_{11}\,[a_{11}\,a_{31} + a_{12}\,a_{32}]^2 + s_{33}\,[a_{13}^2\,a_{33}^2] + \\ & s_{44}\,[a_{13}\,a_{33}][a_{11}\,a_{31} + a_{12}\,a_{32}] + s_{12}\,[a_{11}\,a_{32} - a_{12}\,a_{31}]^2 + \\ & s_{13}\,[a_{33}^2\,[a_{11}^2 + a_{12}^2] + a_{13}^2\,[a_{31}^2 + a_{32}^2]] \end{aligned}$$

Transformation Matrix for General Rotations

Poisson's ratio for the most general case may be derived by considering the transformation matrix for a combination of three coordinate rotations: a first rotation about x_3 by angle φ, a second rotation about the new x_1 by angle θ, and a third rotation about the resulting x_2 by angle ψ. When these angles are set to zero, the x_1, x_2, x_3 axes coincide

respectively with the reference crystallographic directions. For nonzero angles, the direction cosines a_{mn} are as follows:

$$\begin{matrix} [c(\varphi)c(\psi) - s(\varphi)s(\theta)s(\psi)] & [s(\varphi)c(\psi) + c(\varphi)s(\theta)s(\psi)] & [-c(\theta)s(\psi)] \\ [-s(\varphi)c(\theta)] & [c(\varphi)c(\theta)] & [\ s(\theta)\ ] \\ [c(\varphi)s(\psi) + s(\varphi)s(\theta)c(\psi)] & [s(\varphi)s(\psi) - c(\varphi)s(\theta)c(\psi)] & [\ c(\theta)c(\psi)] \end{matrix}$$

Substitution of these a_{mn} into the expressions for s_{11}', s_{12}', and s_{13}', and thence into the formulas $\nu_{21} = s_{12}' / s_{11}'$ and $\nu_{31} = s_{13}' / s_{11}'$ formally solves the problem for specified values of φ, θ, and ψ.

Poisson's Ratios for Specific Orientations

1) Longitudinal extension in the basal plane: $\psi = 0$; φ and θ arbitrary. Direction cosines are:

$$\begin{matrix} [c(\varphi)] & [s(\varphi)] & [0] \\ [-s(\varphi)c(\theta)] & [c(\varphi)c(\theta)] & [s(\theta)] \\ [s(\varphi)s(\theta)] & [-c(\varphi)s(\theta)] & [c(\theta)] \end{matrix}$$

Rotated compliances are independent of angle φ, as required by transverse isotropy:

$$s_{11}' = s_{11}$$

$$s_{12}' = s_{12} \cos^2(\theta) + s_{13} \sin^2(\theta) = s_{12} + (s_{13} - s_{12}) \sin^2(\theta)$$

$$s_{13}' = s_{12} \sin^2(\theta) + s_{13} \cos^2(\theta) = s_{13} - (s_{13} - s_{12}) \sin^2(\theta)$$

Poisson's ratios are:

$$\nu_{21} = [s_{12} + (s_{13} - s_{12}) \sin^2(\theta)] / s_{11}$$

$$\nu_{31} = [s_{13} - (s_{13} - s_{12}) \sin^2(\theta)] / s_{11}$$

2) Longitudinal extension at an angle ψ from the basal plane; the x_2 axis in the basal plane: $\theta = 0$; φ and ψ arbitrary.
Direction cosines are:

$$\begin{matrix} [c(\varphi)c(\psi)] & [s(\varphi)c(\psi)] & [-s(\psi)] \\ [-s(\varphi)] & [c(\varphi)] & [\ 0\ ] \\ [c(\varphi)s(\psi)] & [s(\varphi)s(\psi)] & [\ c(\psi)] \end{matrix}$$

Rotated compliances are:

$$s_{11}' = s_{11}\,[c^4(\psi)] + s_{33}\,[s^4(\psi)] + (s_{44} + 2\,s_{13})\,[c^2(\psi)\,s^2(\psi)]$$

$$s_{12}' = s_{12}\,[c^2(\psi)] + s_{13}\,[s^2(\psi)] = s_{12} + (s_{13} - s_{12})\,[s^2(\psi)]$$

$$s_{13}' = s_{13}\,[c^4(\psi) + s^4(\psi)] + (s_{11} + s_{33} - s_{44})\,[c^2(\psi)\,s^2(\psi)]$$

The Poisson's ratios are: $\nu_{21} = s_{12}' / s_{11}'$; $\nu_{31} = s_{13}' / s_{11}'$.

3) Longitudinal extension out of the basal plane: φ, θ, and ψ arbitrary.
Direction cosines are:

$$\begin{matrix} [c(\varphi)c(\psi) - s(\varphi)s(\theta)s(\psi)] & [s(\varphi)c(\psi) + c(\varphi)s(\theta)s(\psi)] & [-c(\theta)s(\psi)] \\ [-s(\varphi)c(\theta)] & [c(\varphi)c(\theta)] & [\ s(\theta)\ ] \\ [c(\varphi)s(\psi) + s(\varphi)s(\theta)c(\psi)] & [s(\varphi)s(\psi) - c(\varphi)s(\theta)c(\psi)] & [\ c(\theta)c(\psi)] \end{matrix}$$

Rotated compliances are:

$$s_{11}' = s_{11}\,[s^2(\theta)s^2(\psi) + c^2(\psi)]^2 + s_{33}\,[c^4(\theta)s^4(\psi)] + (s_{44} + 2\,s_{13})\,[c^2(\theta)s^2(\psi)][s^2(\theta)s^2(\psi) + c^2(\psi)]$$

$$s_{12}' = (s_{11} + s_{33} - s_{44})[c^2(\theta)s^2(\theta)s^2(\psi)] + s_{12}\,[c^2(\theta)c^2(\psi)] + s_{13}\,[s^2(\theta)c^2(\psi) + s^2(\psi)(c^4(\theta) + s^4(\theta))]$$

$$s_{13}' = (s_{11} + s_{33} - s_{44})[c^4(\theta)c^2(\psi)s^2(\psi)] + s_{12}\,[s^2(\theta)] + s_{13}\,[c^2(\theta)][c^4(\psi) + s^4(\psi) + 2\,s^2(\theta)c^2(\psi)s^2(\psi)]$$

The Poisson's ratios are: $\nu_{21} = s_{12}' / s_{11}'$; $\nu_{31} = s_{13}' / s_{11}'$. These results reduce to those of Case 1) when $\psi = 0$, and to those of Case 2) when $\theta = 0$.

4) Longitudinal extension at an angle ψ from the basal plane: results are independent of angle φ; first rotation about x_2 by angle ψ, followed by a second rotation about x_1 by angle χ.
Direction cosines are:

$$\begin{matrix} [\ c(\psi)\ ] & [\ 0\ ] & [-s(\psi)\ ] \\ [s(\psi)s(\chi)] & [\ c(\chi)] & [\ c(\psi)s(\chi)] \\ [s(\psi)c(\chi)] & [-s(\chi)] & [c(\psi)c(\chi)] \end{matrix}$$

Rotated compliances are:

$$s_{11}' = s_{11}\,[c^4(\psi)] + s_{33}\,[s^4(\psi)] + (s_{44} + 2\,s_{13})\,[c^2(\psi)s^2(\psi)]$$

$$s_{12}' = (s_{11} + s_{33} - s_{44} - 2\,s_{13})[c^2(\psi)s^2(\psi)s^2(\chi)] + s_{12}\,[c^2(\psi)c^2(\chi)] + s_{13}\,[s^2(\chi) + s^2(\psi)c^2(\chi)]$$

$$s_{13}' = (s_{11} + s_{33} - s_{44} - 2\,s_{13})[c^2(\psi)s^2(\psi)c^2(\chi)] + s_{12}\,[c^2(\psi)s^2(\chi)] + s_{13}\,[c^2(\chi) + s^2(\psi)s^2(\chi)]$$

The Poisson's ratios are: $\nu_{21} = s_{12}' / s_{11}'$; $\nu_{31} = s_{13}' / s_{11}'$. These results reduce to those of Case 1) when $\psi = 0$, and to those of Case 2) when $\chi = 0$.

Conclusions

Poisson's ratio, with respect to rotated coordinate axes for hexagonal materials, has been obtained. All results are independent of rotations about the 6-fold axis (angle φ). Two cases are of particular interest:

- For longitudinal extension in the basal plane:
  $\nu_{21} = s_{12} / s_{11}$; $\nu_{31} = s_{13} / s_{11}$
- For longitudinal extension along the 6-fold axis:
  $\nu_{21} = \nu_{31} = s_{13} / s_{33}$

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